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Relations between Cartesian and spherical components of irreducible Cartesian tensors

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Abstract. Explicit formulae which relate Cartesian and spherical components of irreducible Cartesian tensors are derived. For the description of spin-s particles, explicit formulae for the Cartesian tensors and the spherical tensors are given in terms of symmetrised products of spin operators.

1. Introduction

For a long time, nuclear reactions have dealt with polarised spin-$\frac{1}{2}$ and spin-1 particles. For these studies, the Madison convention (1971) recommends the use of two kinds of operators which are either spherical tensors (Lakin 1955) or Cartesian tensors (Goldfarb 1958). With the construction of heavy-ion accelerators, polarised nuclei with higher spin are now available for nuclear reactions. The aim of this work is to extend the two previous kinds of operators to any spin and to study the relations between them.

Section 2 is devoted to the general relations between the Cartesian and the spherical components in the special case of irreducible Cartesian tensors. After a brief recall in § 2.1 of the general Cartesian–spherical transformation, the irreducible Cartesian tensors are defined in § 2.2 and the properties of their components are given. The explicit formulae which relate their Cartesian and spherical components are derived in §§ 2.3 and 2.4.

Section 3 is an application of the previous one to operators belonging to the algebra generated by the spin operators S_x, S_y and S_z associated with the description of a spin-s particle. The definition and some properties of bases of operators which are Cartesian or spherical components of irreducible Cartesian tensors are recalled in § 3.1. An explicit expression for these basis operators in terms of symmetrised products of spin operators is derived in § 3.2. Taking into account the usual normalisations, we give in § 3.3 the expressions for any operator either in terms of a basis of spherical component operators or in terms of an overcomplete set of Cartesian component operators. The relation between these latter operators can be taken into account to express any operator in terms of a minimum set of linear combinations of Cartesian component operators. A simple way to do this is explained.

Finally, in the conclusion we discuss the use of these three kinds of expansions for any operator in the description of nuclear reactions. It is then shown that the spherical component operators are the easiest to handle.

Large tables of coefficients are given for applications, although these coefficients are easy to obtain from explicit formulae except for the Tchebichef polynomials for which we used a computer.

2. Cartesian–spherical transformations for irreducible Cartesian tensors

2.1. General formulation of Cartesian–spherical transformations

With respect to the three-dimensional rotation group, a tensor (Normand 1980) $T = T^{1\ldots1}$ of order l and with each of its l ranks equal to one is defined by 3^l components which belong to an associative but not necessarily commutative algebra over the complex field $\mathbb{C}$. The Cartesian components $(T_{i_1\ldots i_l};\, i_k = x, y, z)$ and the spherical components $(T^{1\ldots1}_{m_1\ldots m_l};\, m_k = 1, 0, -1)$ are characterised by their law of transformation:

$$R = (R^{i'}_{i}) \in \mathrm{SO}(3) \qquad {}^{R}T_{i_1\ldots i_l} = \sum_{i'_1,\ldots,i'_l} T_{i'_1\ldots i'_l} \prod_{k=1}^{l} R^{i'_k}_{i_k} \tag{1a}$$

$${}^{R}T^{1\ldots1}_{m_1\ldots m_l} = \sum_{m'_1,\ldots,m'_l} T^{1\ldots1}_{m'_1\ldots m'_l} \prod_{k=1}^{l} \mathscr{D}^{1}_{m'_k m_k}(R) \tag{1b}$$

where $\mathscr{D}^1(R)$ is the irreducible rotation matrix for spin one. Since, up to an equivalence, $\mathscr{D}^1$ is the only unitary and irreducible three-dimensional representation of SO(3), the Cartesian and spherical components are related by

$$T^{1\ldots1}_{m_1\ldots m_l} = \sum_{i_1,\ldots,i_l} T_{i_1\ldots i_l} \prod_{k=1}^{l} \langle i_k|1m_k\rangle \tag{2a}$$

$$T_{i_1\ldots i_l} = \sum_{m_1,\ldots,m_l} T^{1\ldots1}_{m_1\ldots m_l} \prod_{k=1}^{l} \langle 1m_k|i_k\rangle \tag{2b}$$

where the matrix $(\langle i|1m\rangle)$ is a multiple of a unitary matrix:

$$\begin{array}{cc} & \begin{array}{ccc} 1 & 0 & -1 \end{array} \\ (\langle i|1m\rangle) = c & \begin{pmatrix} -1/\sqrt{2} & 0 & 1/\sqrt{2} \\ -\mathrm{i}/\sqrt{2} & 0 & -\mathrm{i}/\sqrt{2} \\ 0 & 1 & 0 \end{pmatrix} \begin{array}{c} x \\ y \\ z \end{array} \end{array} \qquad c \in \mathbb{C}. \tag{3}$$

As is usual, we will assume from now on that

$$c^2 = \pm 1 \qquad \text{i.e. } c = \pm 1 \text{ or } \pm \mathrm{i}; \tag{4}$$

e.g. $c = 1$ in the Madison convention (1971), Edmonds (1968) and Normand and Raynal (1981), $c = \mathrm{i}$ in Fano and Racah (1959) and $c = \mathrm{i}\kappa$ in Stone (1975, 1976). The matrix $(\langle i|1m\rangle)$ is then unitary:

$$\langle i|1m\rangle^* = \langle 1m|i\rangle. \tag{5}$$

A further property reads

$$\langle i|1m\rangle^* = c^{-2}(-1)^m \langle i|1-m\rangle. \tag{6}$$

Therefore, if the Cartesian components are real quantities or Hermitian operators, one gets

$$T^{1\ldots1\,*\,\mathrm{or}\,+}_{m_1\ldots m_l} = c^{-2l}(-1)^{\Sigma_{k=1}^{l} m_k} T^{1\ldots1}_{-m_1\ldots-m_l}. \tag{7}$$

Any tensor $T^{1\ldots1}$ of order l greater than one can be decomposed into irreducible tensors $T^{(1\ldots1,\lambda\alpha)j}$ of integer rank j, $0 \le j \le l$, and characterised by a coupling scheme specified by $l-2$ intermediate couplings $\lambda = (\lambda_k;\, k = 1, \ldots, l-2)$ and their order symbolically denoted by α. One then defines a transformation

$$T^{\{1\ldots 1,\lambda\alpha\}j}_{m} = \sum_{i_1,\ldots,i_l} T_{i_1\ldots i_l}\langle i_1\ldots i_l|\lambda\alpha, jm\rangle \tag{8}$$

where

$$\langle i_1\ldots i_l|\lambda\alpha, jm\rangle = \sum_{m_1,\ldots,m_l} C_{\lambda\alpha}{}^{1\ \ldots\ 1\ \ j}_{m_1\ldots m_l m} \prod_{k=1}^{l} \langle i_k|1m_k\rangle, \tag{9}$$

the coupling coefficients $C_{\lambda\alpha}{}^{1\ \ldots\ 1\ \ j}_{m_1\ldots m_l m}$ being products of $l-1$ Clebsch–Gordan coefficients. From the orthogonality relations of Clebsch–Gordan coefficients, the inverse transformation of equation (8) reads, for a given α,

$$T_{i_1\ldots i_l} = \sum_{\lambda,j,m} T^{\{1\ldots 1,\lambda\alpha\}j}_{m}\langle\lambda\alpha, jm|i_1\ldots i_l\rangle \tag{10}$$

where

$$\langle\lambda\alpha, jm|i_1\ldots i_l\rangle = \sum_{m_1,\ldots,m_l} C_{\lambda\alpha}{}^{1\ \ldots\ 1}_{m_1\ldots m_l} \prod_{k=1}^{l}\langle 1m_k|i_k\rangle. \tag{11}$$

From equation (5) the transformation above is unitary:

$$\langle i_1\ldots i_l|\lambda\alpha, jm\rangle^* = \langle\lambda\alpha, jm|i_1\ldots i_l\rangle. \tag{12}$$

A further property follows from equation (6) and the symmetry of Clebsch–Gordan coefficients under the change of sign of all indices m_k, μ_k and m, namely

$$\langle i_1\ldots i_l|\lambda\alpha, jm\rangle^* = c^{-2l}(-1)^{l-j+m}\langle i_1\ldots i_l|\lambda\alpha, j-m\rangle. \tag{13}$$

Thus, under the same conditions as for equation (7), one finds

$$T^{\{1\ldots 1,\lambda\alpha\}j*\text{or}+}_{m} = c^{-2l}(-1)^{l-j+m}T^{\{1\ldots 1,\lambda\alpha\}j}_{m}. \tag{14}$$

2.2. *Irreducible Cartesian tensors*

Attention is now focused on the couplings to the highest value l of j, and the following is shown:

(i) The coefficients $\langle i_1\ldots i_l|\lambda\alpha, lm\rangle$ are independent of the coupling scheme $\lambda\alpha$, and invariant under any permutation of the indices i_k. Hence, they will henceforth be denoted by

$$\langle pqr|lm\rangle = \langle i_1\ldots i_l|\lambda\alpha, lm\rangle \tag{15}$$

where the indices x, y and z occur, respectively, p, q and r times in $i_1\ldots i_l$ ($p+q+r=l$).

(ii) The contraction of any two Cartesian indices i_a and i_b leads to

$$\sum_{i_a,i_b}\langle i_1\ldots i_a\ldots i_b\ldots i_l|\lambda\alpha, lm\rangle\delta_{i_a i_b}$$

$$= \langle p'+2\,q'r'|lm\rangle + \langle p'q'+2\,r'|lm\rangle + \langle p'q'r'+2|lm\rangle = 0 \tag{16}$$

where $p'+q'+r'=l-2$.

These properties are based on the independence of the coupling coefficients with j equal to the highest value l with respect to the coupling scheme. Indeed, for two orders of couplings one has *a priori*

$$C_{\lambda\alpha}{}^{1\ \ldots\ 1\ \ l}_{m_1\ldots m_l m} = \sum_{\lambda'} C_{\lambda'\alpha'}{}^{1\ \ldots\ 1\ \ l}_{m_1\ldots m_l m} R(\lambda\alpha, \lambda'\alpha', lm) \tag{17}$$

where the recoupling coefficients $R(\lambda\alpha, \lambda'\alpha', lm)$ are multiples of $3(l-1)j$ symbols. It follows from the Wigner–Eckart theorem that these latter coefficients are independent of m; hence, setting $m = l$ yields $R(\lambda\alpha, \lambda'\alpha', lm) = 1$ as a product of $2(l-1)$ Clebsch–Gordan coefficients all equal to one. Moreover, due to the coupling to the highest value l, the sum over the intermediate couplings λ' in (17) contains only one term (QED). One can then use the step-by-step coupling scheme considered by Stone (1975), and apply his results to the special coupling to the highest value l. Let us nevertheless give a straightforward proof of properties (i) and (ii). The $C_{\lambda\alpha\, m_1\; m_l\, m}^{\;\;\;1\,\dots\,1\;\; l}$ are invariant under any permutation of the indices m_k, since this corresponds to a special change of the coupling scheme. Property (i) then arises from equation (9). Choosing in equation (16) a coupling scheme where the ath and the bth spins one are coupled together necessarily to two, one finds, using equations (5) and (6),

$$\sum_{i_a, i_b} \delta_{i_a i_b} \langle i_1 \dots i_a \dots i_b \dots i_l | lm \rangle \propto \sum_{i_a, i_b, m_a, m_b} \langle 1 1 m_a m_b | 2\mu \rangle \langle i_a | 1 m_a \rangle \langle i_b | 1 m_b \rangle \delta_{i_a i_b}$$

$$= c^{-2}\sqrt{3} \sum_{m_a, m_b} \langle 1 1 m_a m_b | 2\mu \rangle \langle 1 1 m_a m_b | 00 \rangle \tag{18}$$

where only the relevant terms are explicitly written. Property (ii) then follows from the orthogonality relations of Clebsch–Gordan coefficients.

An explicit expression and some properties of coefficients $\langle pqr | lm \rangle$ are derived below in § 2.4.

By definition, an irreducible Cartesian tensor, also said to be in natural form (Coope *et al* 1965), is a tensor of order l with l ranks one, such that all its irreducible tensors vanish except the one with the highest rank l, denoted from now on by $(T_l)^l$. The previously derived properties of $\langle pqr | lm \rangle$ imply that such a tensor T_l is completely symmetrical and traceless: namely, from equations (9), (12) and (15), its Cartesian components $(T_l)_{i_1 \dots i_l}$ are invariant under any permutation of indices $i_1 \dots i_l$, and they will henceforth be denoted by

$$(T_l)_{pqr} = (T_l)^l_m \langle lm | pqr \rangle \qquad p+q+r = l. \tag{19}$$

Furthermore, equation (16) yields

$$(T_l)_{p'+2\, q' r'} + (T_l)_{p' q'+2\, r'} + (T_l)_{p' q' r'+2} = 0 \qquad p'+q'+r' = l-2, \tag{20}$$

which means that T_l is traceless on contraction of any pair of Cartesian indices. Actually, T_l is characterised by the two properties above (Coope *et al* 1965). An irreducible Cartesian tensor T_l has $2l+1$ linearly independent components $(T_l)^l_m$. Therefore, its 3^l Cartesian components are not independent for $l \geqslant 2$: on the one hand they are completely symmetrical and thus there are

$$n_l = \tfrac{1}{2}(l+1)(l+2) \tag{21}$$

components $(T_l)_{pqr}$; and on the other hand they have to satisfy the n_{l-2} relations (20). One thus recovers the proper number of linearly independent components for

$$2l+1 = n_l - n_{l-2}. \tag{22}$$

2.3. Spherical components in terms of the Cartesian ones

Since $n_l > 2l+1$ for $l \geqslant 2$, the expression for the spherical components of T_l in terms of its Cartesian components arising from equation (8), i.e.

$$(T_l)^l_m = \sum_{\substack{p,q,r\\p+q+r=l}} \frac{l!}{p!\,q!\,r!}(T_l)_{pqr}\langle pqr|lm\rangle, \tag{23}$$

is not unique. The extra factor $l!/p!\,q!\,r!$ is the number of sequences of Cartesian indices $i_1 \ldots i_l$ which correspond to given values of p, q and r. Taking advantage of this freedom, one now derives a minimal expansion for the spherical components

$$(T_l)^l_m = \sum_{\substack{p,q,r\\p+q+r=l}} (T_l)_{pqr}(pqr|lm) \tag{24}$$

where minimal means that each $(T_l)^l_m$ is expressed in terms of the smallest number of Cartesian components, and the $(pqr|lm)$ are coefficients determined below.

Being completely symmetrical, the components $(T_l)_{pqr}$ behave under the rotation group as the monomials $x^p y^q z^r$. From equations (2a) and (3) one thus has

$$(T_l)^l_l = T^{1\ldots1}_{1\ldots1} \approx \left(\frac{-c}{\sqrt{2}}(x+\mathrm{i}y)\right)^l = c^l l!\left(\frac{4\pi 2^l}{(2l+1)(2l)!}\right)^{1/2} \mathcal{Y}_{ll}(\rho, \vartheta, \varphi) \tag{25}$$

where $\approx$ means that a monomial $x^p y^q z^r$ stands for $(T_l)_{pqr}$, and $\mathcal{Y}_{lm}(\rho, \vartheta, \varphi)$ is a solid harmonics with

$$x = \rho \sin\vartheta \cos\varphi \qquad y = \rho \sin\vartheta \sin\varphi \qquad z = \rho\cos\vartheta. \tag{26}$$

The components $(T_l)^l_m$ are obtained by a repeated action of the infinitesimal generator J_- of the representation considered, which amounts to applying

$$j_- = (x - \mathrm{i}y)\frac{\partial}{\partial z} - 2z\frac{\partial}{\partial(x+\mathrm{i}y)} \tag{27}$$

on the right-hand side of equation (25), yielding

$$(T_l)^l_m \approx c^l l!\left(\frac{4\pi 2^l}{(2l+1)(2l)!}\right)^{1/2} \mathcal{Y}_{lm}(\rho, \vartheta, \varphi). \tag{28}$$

In terms of monomials the constraints (20) read

$$x^2 + y^2 + z^2 = 0. \tag{29}$$

Taking into account this relation in the expression for $\mathcal{Y}_{lm}$, the minimum number of monomials $x^p y^q z^r$ is then obtained by replacing the two monomials $x^2 + y^2$ by the single one $-z^2$. Since

$$x^2 + y^2 = \rho^2 - \rho^2\cos^2\vartheta \qquad -z^2 = -\rho^2\cos^2\vartheta, \tag{30}$$

the above procedure amounts to taking in $\mathcal{Y}_{lm}$ only the coefficient of the highest degree in $\cos\vartheta$. One thereby finds

$$(T_l)^l_{\pm|m|} \approx c^l\left(\frac{(2l)!}{2^l(l-m)!(l+m)!}\right)^{1/2} [\mp(x+\mathrm{i}y)]^{|m|} z^{l-|m|} \tag{31}$$

(cf table 1 for $l \leqslant 4$) and finally

$$(T_l)^l_{\pm|m|} = c^l\left(\frac{(2l)!}{2^l(l-m)!(l+m)!}\right)^{1/2} (\mp 1)^m \sum_{\mu=0}^{|m|} (\pm\mathrm{i})^\mu \binom{|m|}{\mu} (T_l)_{|m|-\mu\, \mu\, l-|m|} \tag{32a}$$

Table 1. Spherical components $(T_l)^l_m$ of an irreducible Cartesian tensor T_l in terms of its Cartesian components $(T_l)_{pqr}$, here denoted by $x^py^qz^r$, equation (31). The coefficient c_l occurs in the relation between the $(T_l)^l_m$ and the solid harmonics, equation (28).

l	m	$c^{-l}(T_l)^l_m$	$c_l = l!\left(\frac{2}{(2l+1)(2l)!}\right)^{1/2}$
0	0	1	1
1	±1	$\mp\frac{1}{\sqrt{2}}(x\pm iy)$	$\frac{1}{\sqrt{3}}$
	0	z	
2	±2	$\frac{1}{2}(x^2\pm2ixy-y^2)$	$\sqrt{\frac{2}{15}}$
	±1	$\mp(xz\pm iyz)$	
	0	$\sqrt{\frac{3}{2}}\,z^2$	
3	±3	$\mp\frac{1}{2\sqrt{2}}(x^3\pm3ix^2y-3xy^2\mp iy^3)$	$\sqrt{\frac{2}{35}}$
	±2	$\frac{\sqrt{3}}{2}(x^2z\pm2ixyz-y^2z)$	
	±1	$\mp\frac{1}{2}\sqrt{\frac{15}{2}}(xz^2\pm iyz^2)$	
	0	$\sqrt{\frac{5}{2}}\,z^3$	
4	±4	$\frac{1}{4}(x^4\pm4ix^3y-6x^2y^2\mp4ixy^3+y^4)$	$\frac{2}{3}\sqrt{\frac{2}{35}}$
	±3	$\mp\frac{1}{\sqrt{2}}(x^3z\pm3ix^2yz-3xy^2z\mp iy^3z)$	
	±2	$\frac{\sqrt{7}}{2}(x^2z^2\pm2ixyz^2-y^2z^2)$	
	±1	$\mp\sqrt{\frac{7}{2}}(xz^3\pm iyz^3)$	
	0	$\frac{1}{2}\sqrt{\frac{35}{2}}\,z^4$	

$$(pqr|l\pm|m|) = c^l(-1)^m(\pm1)^p i^q\left(\frac{(2l)!}{2^l(l-m)!(l+m)!}\right)^{1/2}\frac{(p+q)!}{p!q!}\delta_{p+q,|m|}\delta_{r,l-|m|}. \qquad (32b)$$

The same results can be obtained from

$$(T_l)^l_m \approx (-c)^l\left(\frac{(l+m)!}{2^l(2l)!(l-m)!}\right)^{1/2} j_-^{l-m}(x+iy)^l, \qquad (33)$$

where, using equation (27), $j_-^{l-m}(x+iy)^l$ is computed recursively, replacing at each step $(x+iy)(x-iy)$ by $-z^2$ to take into account equation (29).

It follows from equation (14), or directly from equation (32b), that the coefficients $(pqr|lm)$ satisfy

$$(pqr|lm)^* = c^{-2l}(-1)^m(pqr|l-m), \qquad (34)$$

and a further property reads

$$(pqr|l-m) = (-1)^p(pqr|lm). \qquad (35)$$

2.4. *Cartesian components in terms of the spherical ones*

The analogy between the monomials $x^py^qz^r$ $(p+q+r=l)$ and the Cartesian components $(T_l)_{pqr}$ provides us with a method of computing the coefficients $\langle lm|pqr\rangle$ which occur in equation (19). The expansion of $x^py^qz^r$ in terms of monomials

$(x+\mathrm{i}y)^s(x-\mathrm{i}y)^t z^r$ reads

$$(T_l)_{pqr} \approx (-\mathrm{i})^q \frac{1}{2^{p+q}} \sum_{k=0}^{p+q} \sum_j \frac{(-1)^j p!\,q!}{j!\,(k-j)!\,(p-k+j)!\,(q-j)!} (x+\mathrm{i}y)^{p+q-k}(x-\mathrm{i}y)^k z^r. \tag{36}$$

Replacing $(x+\mathrm{i}y)(x-\mathrm{i}y)$ by $-z^2$ to take into account equation (29), and using equation (31), it becomes

$$(x+\mathrm{i}y)^{p+q-k}(x-\mathrm{i}y)^k z^r \approx c^{-l}(-1)^{p+q-k}\left(\frac{2^l(l-m)!(l+m)!}{(2l)!}\right)^{1/2} (T_l)^l_m \tag{37}$$

where

$$m = p+q-2k. \tag{38}$$

Therefore, we obtain

$$\begin{aligned}\langle lm|pqr\rangle &= \langle pqr|lm\rangle^* \\ &= c^{-l}\mathrm{i}^q\left(2^{r-p-q}\frac{(l-m)!(l+m)!}{(2l)!}\right)^{1/2} C(p,q,m)\frac{1-(-1)^{p+q+m}}{2}\delta_{l,p+q+r}\end{aligned} \tag{39}$$

with

$$\begin{aligned}C(p,q,m) &= \sum_j \frac{(-1)^j p!\,q!}{j!\,(p-j)![\frac{1}{2}(p+q+m)-j]![\frac{1}{2}(q-p-m)+j]!} \\ &= \frac{q!}{[\frac{1}{2}(p+q+m)]![\frac{1}{2}(q-p-m)]!} \\ &\quad \times {}_2F_1[-p, -\tfrac{1}{2}(p+q+m); \tfrac{1}{2}(q-p-m)+1; -1].\end{aligned} \tag{40}$$

The value of the quantity $C(p,q,m)$ above is given in table 2 for constant $p+q \leqslant 8$.

Let us now derive some properties of coefficients $\langle lm|pqr\rangle$.

Symmetry relations. From equation (38) these coefficients vanish for $p+q+m$ odd. Furthermore, the symmetries of hypergeometric series imply

$$C(p,q,m) = (-1)^{(p+q+m)/2}C(q,p,m) = (-1)^p C(p,q,-m) \tag{41}$$

which yields

$$\langle lm|pqr\rangle = (-1)^{(p+q+m)/2}\mathrm{i}^{q-p}\langle lm|qpr\rangle = (-1)^p\langle l-m|pqr\rangle. \tag{42}$$

In particular, these relations induce

$$\langle lm|ppr\rangle = 0 \qquad \text{if } p+\tfrac{1}{2}m \text{ odd} \tag{43}$$

$$\langle l0|pqr\rangle = 0 \qquad \text{if } p \text{ odd}. \tag{44}$$

Furthermore, it is recalled that the coefficients $\langle lm|pqr\rangle$ satisfy equation (13), i.e.

$$\langle lm|pqr\rangle^* = c^{2l}(-1)^m\langle l-m|pqr\rangle, \tag{45}$$

as can be checked directly from equation (39).

Generating function. Setting

$$x+\mathrm{i}y = u \qquad x-\mathrm{i}y = -1/u \qquad z=1 \tag{46}$$

Table 2. Cartesian components $(T_l)_{pqr}$ of an irreducible Cartesian tensor T_l in terms of the A_{lm}^{ϵ}, equation (51). The factor in front of each A_{lm}^{ϵ} of this table is equal to $C(p,q,m)$, equation (40).

p	q	r	$c^l(-\mathrm{i})^q 2^{p+q}(T_l)_{pqr}$
0	0	l	A_{l0}^{1}
1	0	$l-1$	$-A_{l1}^{-1}$
0	1		A_{l1}^{1}
2	0	$l-2$	$A_{l2}^{1}-2A_{l0}^{1}$
1	1		$-A_{l2}^{-1}$
0	2		$A_{l2}^{1}+2A_{l0}^{1}$
3	0	$l-3$	$-A_{l3}^{-1}+3A_{l1}^{-1}$
2	1		$A_{l3}^{1}-A_{l1}^{1}$
1	2		$-A_{l3}^{-1}-A_{l1}^{-1}$
0	3		$A_{l3}^{1}+3A_{l1}^{1}$
4	0	$l-4$	$A_{l4}^{1}-4A_{l2}^{1}+6A_{l0}^{1}$
3	1		$-A_{l4}^{-1}+2A_{l2}^{-1}$
2	2		$A_{l4}^{1}-2A_{l0}^{1}$
1	3		$-A_{l4}^{-1}-2A_{l2}^{-1}$
0	4		$A_{l4}^{1}+4A_{l2}^{1}+6A_{l0}^{1}$
5	0	$l-5$	$-A_{l5}^{-1}+5A_{l3}^{-1}-10A_{l1}^{-1}$
4	1		$A_{l5}^{1}-3A_{l3}^{1}+2A_{l1}^{1}$
3	2		$-A_{l5}^{-1}+A_{l3}^{-1}+2A_{l1}^{-1}$
2	3		$A_{l5}^{1}+A_{l3}^{1}-2A_{l1}^{1}$
1	4		$-A_{l5}^{-1}-3A_{l3}^{-1}-2A_{l1}^{-1}$
0	5		$A_{l5}^{1}+5A_{l3}^{1}+10A_{l1}^{1}$
6	0	$l-6$	$A_{l6}^{1}-6A_{l4}^{1}+15A_{l2}^{1}-20A_{l0}^{1}$
5	1		$-A_{l6}^{-1}+4A_{l4}^{-1}-5A_{l2}^{-1}$
4	2		$A_{l6}^{1}-2A_{l4}^{1}-A_{l2}^{1}+4A_{l0}^{1}$
3	3		$-A_{l6}^{-1}+3A_{l2}^{-1}$
2	4		$A_{l6}^{1}+2A_{l4}^{1}-A_{l2}^{1}-4A_{l0}^{1}$
1	5		$-A_{l6}^{-1}-4A_{l4}^{-1}-5A_{l2}^{-1}$
0	6		$A_{l6}^{1}+6A_{l4}^{1}+15A_{l2}^{1}+20A_{l0}^{1}$
7	0	$l-7$	$-A_{l7}^{-1}+7A_{l5}^{-1}-21A_{l3}^{-1}+35A_{l1}^{-1}$
6	1		$A_{l7}^{1}-5A_{l5}^{1}+9A_{l3}^{1}-5A_{l1}^{1}$
5	2		$-A_{l7}^{-1}+3A_{l5}^{-1}-A_{l3}^{-1}-5A_{l1}^{-1}$
4	3		$A_{l7}^{1}-A_{l5}^{1}-3A_{l3}^{1}+3A_{l1}^{1}$
3	4		$-A_{l7}^{-1}-A_{l5}^{-1}+3A_{l3}^{-1}+3A_{l1}^{-1}$
2	5		$A_{l7}^{1}+3A_{l5}^{1}+A_{l3}^{1}-5A_{l1}^{1}$
1	6		$-A_{l7}^{-1}-5A_{l5}^{-1}-9A_{l3}^{-1}-5A_{l1}^{-1}$
0	7		$A_{l7}^{1}+7A_{l5}^{1}+21A_{l3}^{1}+35A_{l1}^{1}$
8	0	$l-8$	$A_{l8}^{1}-8A_{l6}^{1}+28A_{l4}^{1}-56A_{l2}^{1}+70A_{l0}^{1}$
7	1		$-A_{l8}^{-1}+6A_{l6}^{-1}-14A_{l4}^{-1}+14A_{l2}^{-1}$
6	2		$A_{l8}^{1}-4A_{l6}^{1}+4A_{l4}^{1}+4A_{l2}^{1}-10A_{l0}$
5	3		$-A_{l8}^{-1}+2A_{l6}^{-1}+2A_{l4}^{-1}-6A_{l2}^{-1}$
4	4		$A_{l8}^{1}-4A_{l4}^{1}+6A_{l0}^{1}$
3	5		$-A_{l8}^{-1}-2A_{l6}^{-1}+2A_{l4}^{-1}+6A_{l2}^{-1}$
2	6		$A_{l8}^{1}+4A_{l6}^{1}+4A_{l4}^{1}-4A_{l2}^{1}-10A_{l0}^{1}$
1	7		$-A_{l8}^{-1}-6A_{l6}^{-1}-14A_{l4}^{-1}-14A_{l2}^{-1}$
0	8		$A_{l8}^{1}+8A_{l6}^{1}+28A_{l4}^{1}+56A_{l2}^{1}+70A_{l0}^{1}$

in $x^p y^q z^r$ to take into account the relation (29), one gets, on comparing with equations (36) and (39), a generating function

$$F_{pqr}(u) = c^{-l}(-1)^p \mathrm{i}^q \left(\frac{2^{r-p-q}}{(2l)!}\right)^{1/2} \left(u - \frac{1}{u}\right)^p \left(u + \frac{1}{u}\right)^q$$

$$= \sum_{\substack{m=-(p+q) \\ p+q+m \text{ even}}}^{p+q} \frac{u^m}{[(l-m)!(l+m)!]^{1/2}} \langle lm|pqr\rangle \tag{47}$$

with $p+q+r=l$ always. This generating function allows us to check the unitary character of the Cartesian–spherical transformation in the special case considered. Indeed, one establishes

$$\sum_{p,q,r=0}^{\infty} \frac{(p+q+r)!}{p!q!r!} F_{pqr}(u) F^*_{pqr}(u') = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{(uu')^m}{(l-m)!(l+m)!} \tag{48}$$

which yields

$$\sum_{\substack{p,q,r \\ p+q+r=l}} \frac{l!}{p!q!r!} \langle lm|pqr\rangle \langle lm'|pqr\rangle^* = \delta_{mm'}. \tag{49}$$

Special value. It arises from equations (39) and (40) that

$$\langle lm|00l'\rangle = c^{-l}(\sqrt{2})^l \frac{l!}{\sqrt{(2l)!}} \delta_{ll'} \delta_{m0}. \tag{50}$$

Taking advantage of equation (42), the expression (19) for the Cartesian components $(T_l)_{pqr}$ in terms of the spherical components $(T_l)^l_m$ can be rewritten as

$$(T_l)_{pqr} = c^{-l} \frac{\mathrm{i}^q}{2^{p+q}} \sum_{\substack{m=0 \\ p+q+m \text{ even}}}^{p+q} C(p, q, m) A_{lm}^{(-1)^p} \tag{51}$$

where

$$A^{\varepsilon}_{lm} = \frac{1}{1+\delta_{m0}} \left(\frac{2^l (l-m)!(l+m)!}{(2l)!}\right)^{1/2} [(T_l)^l_m + \varepsilon (T_l)^l_{-m}] \tag{52}$$

with $\varepsilon = \pm 1$ and as always $l = p+q+r$. These expressions for $(T_l)_{pqr}$ are listed in table 2 for $p+q \leqslant 8$.

Since A^{-1}_{l0} vanishes, there are $2l+1$ linearly independent objects $\{A^1_{l0}, A^{\varepsilon}_{lm};\ m = 1, \ldots, l,\ \varepsilon = \pm 1\}$ which can be considered instead of the $2l+1$ spherical components $(T_l)^l_m$. Using the minimal expansion (24) for the $(T_l)^l_m$, the A^{ε}_{lm} read, in terms of the Cartesian components $(T_l)_{pqr} \approx x^p y^q z^r$,

$$A^{\varepsilon}_{lm} \approx c^l (-1)^m \sum_{\mu=0}^{m} \mathrm{i}^{\mu} \binom{m}{\mu} \frac{1+\varepsilon(-1)^{m+\mu}}{1+\delta_{m0}} x^{m-\mu} y^{\mu} z^{l-m} \qquad m \geqslant 0. \tag{53}$$

Actually, instead of the A^{ε}_{lm} one usually considers proportional quantities normalised in such a way that the coefficient of the monomial with the highest degree in x, i.e. forgetting z, x^m or $x^{m-1}y$, be one, except if there exists a monomial y^m and no monomial x^m in which case the coefficient of y^m is taken equal to one. Casting the dependence upon z aside, one then defines polynomials B_m^ε in x and y, distinguishing four cases:

$$A_{lm}^\varepsilon \approx c^l f_m^\varepsilon B_m^\varepsilon z^{l-m} \tag{54a}$$

$$f_{2n}^1 = \frac{2}{1+\delta_{n0}} \qquad B_{2n}^1 = \sum_{\nu=0}^{n} (-1)^\nu \binom{2n}{2\nu} x^{2n-2\nu} y^{2\nu} \qquad n = 0, 1, \ldots \tag{54b}$$

$$f_{2n}^{-1} = 4n\mathrm{i} \qquad B_{2n}^{-1} = \frac{1}{2n} \sum_{\nu=0}^{n-1} (-1)^\nu \binom{2n}{2\nu+1} x^{2n-2\nu-1} y^{2\nu+1} \qquad n = 1, 2, \ldots \tag{54c}$$

$$f_{2n+1}^1 = 2\mathrm{i}(-1)^{n+1} \qquad B_{2n+1}^1 = (-1)^n \sum_{\nu=0}^{n} (-1)^\nu \binom{2n+1}{2\nu+1} x^{2n-2\nu} y^{2\nu+1} \qquad n = 0, 1, \ldots \tag{54d}$$

$$f_{2n+1}^{-1} = -2 \qquad B_{2n+1}^{-1} = \sum_{\nu=0}^{n} (-1)^\nu \binom{2n+1}{2\nu} x^{2n+1-2\nu} y^{2\nu} \qquad n = 0, 1, \ldots. \tag{54e}$$

These polynomials B_m^ε are listed in table 3 for $l \leqslant 6$.

Table 3. Polynomials B_m^ε in x and y which occur in the minimal expansion of the A_{lm}^ε in terms of the spherical components $(T_l)_{pqr}$, here denoted by $x^p y^q z^r$, equations (54*b*–*e*).

m	ε	B_m^ε
0	1	1
1	1	y
	-1	x
2	1	$x^2 - y^2$
	-1	xy
3	1	$y^3 - 3x^2y$
	-1	$x^3 - 3xy^2$
4	1	$x^4 - 6x^2y^2 + y^4$
	-1	$x^3y - xy^3$
5	1	$y^5 - 10x^2y^3 + 5x^4y$
	-1	$x^5 - 10x^3y^2 + 5xy^4$
6	1	$x^6 - 15x^4y^2 + 15x^2y^4 - y^6$
	-1	$x^5y - \frac{10}{3}x^3y^3 + xy^5$

3. Tensors built with spin operators

3.1. Description of a spin-s particle

To describe a spin-s particle one considers the algebra $\mathscr{A}_s$ over the complex field of operators A, functions of the fundamental observables S_i ($i = x, y, z$) which satisfy the commutation relations of angular momenta:

$$[S_i, S_j] = \mathrm{i}\varepsilon_{ijk} S_k. \tag{55}$$

These operators act in the $(2s+1)$-dimensional space $\mathscr{H}_s$ spanned by the orthonormal basis $(|s\mu\rangle;\ \mu = s, s-1, \ldots, -s)$ which forms a standard basis of the representation of the rotation group on $\mathscr{H}_s$:

$$(S_x \pm \mathrm{i}S_y)|s\mu\rangle = \sqrt{(s \mp \mu)(s \pm \mu + 1)}|s\mu \pm 1\rangle \qquad S_z|s\mu\rangle = \mu|s\mu\rangle \tag{56a}$$

$$S_x^2 + S_y^2 + S_z^2 = s(s+1)\mathbf{1}. \tag{56b}$$

The operators A in $\mathscr{A}_s$ transform under the rotation group according to the adjoint representation, the infinitesimal generators of which are defined by

$$J_i A = [S_i, A]. \tag{57}$$

The algebra $\mathscr{A}_s$ is spanned by the $(2s+1)^2$ uncoupled generalised projection operators $|s\mu\rangle\langle s\mu'|$, which are orthogonal in the following way:

$$\mathrm{Tr}[|s\mu\rangle\langle s\mu'|(|s\nu\rangle\langle s\nu'|)^+] = \delta_{\mu\nu}\delta_{\mu'\nu'}. \tag{58}$$

Therefore, any operator A in $\mathscr{A}_s$, especially the density operator associated with the description of any physical state, can be expressed as

$$A = \sum_{\mu,\mu'} |s\mu\rangle\langle s\mu'|\,\mathrm{Tr}[A(|s\mu\rangle\langle s\mu'|)^+] = \sum_{\mu,\mu'} |s\mu\rangle\langle s\mu|A|s\mu'\rangle\langle s\mu'|. \tag{59}$$

Since we are interested in the behaviour of operators under the rotation group, it is convenient to define irreducible tensor operators which are proportional to coupled generalised projection operators (Raynal 1964, 1972):

$$T_{sm}^{\,l} = a_{sl} \sum_{\mu,\mu'} (-1)^{s-\mu'}\langle ss\mu - \mu'|lm\rangle|s\mu\rangle\langle s\mu'| \qquad \begin{matrix} l = 0, 1, \ldots, 2s \\ m = l, l-1, \ldots, -l \end{matrix} \tag{60a}$$

$$|s\mu\rangle\langle s\mu'| = (-1)^{s-\mu'} \sum_{l,m} \frac{1}{a_{sl}}\langle ss\mu - \mu'|lm\rangle T_{sm}^{\,l} \tag{60b}$$

where the a_{sl} are non-zero complex normalisation coefficients to be chosen. In terms of the notations for the tensorial character specified by Normand (1980), one has, from equations (11.12) and (11.13),

$$|s\mu\rangle\langle s\mu'| = P^{[s](s)}_{\mu\ \mu'} \tag{61a}$$

$$T_{sm}^{\,l} = a_{sl}(-1)^{2s}c_s P^{(ss)[l]}_{\ \ m}. \tag{61b}$$

The operators $T_{sm}^{\,l}$ span the algebra $\mathscr{A}_s$, and it follows from the orthogonality relation of Clebsch–Gordan coefficients that they are also orthogonal according to

$$\mathrm{Tr}(T_{sm}^{\,l} T_{sm'}^{\,l'+}) = |a_{sl}|^2\delta_{ll'}\delta_{mm'}. \tag{62}$$

Any operator A in $\mathscr{A}_s$, e.g. a density operator, then reads

$$A = \sum_{l,m} T_{sm}^{\,l} \frac{1}{|a_{sl}|^2}\mathrm{Tr}(AT_{sm}^{\,l+}). \tag{63}$$

One should notice that

$$T_{sm}^{\,l+} = \frac{a_{sl}^{\;*}}{a_{sl}}(-1)^m T_{s-m}^{\,l}. \tag{64}$$

As is usual (Madison convention 1971), one from now on chooses

$$a_{sl} = c^l\sqrt{2s+1} \tag{65}$$

where the factor c is identical to the one considered previously, equation (4). One then has

$$T_{s0}^{0}=\mathbf{1} \tag{66a}$$

$$T_{sm}^{l+}=c^{-2l}(-1)^{m}T_{s-m}^{l} \tag{66b}$$

$$\mathrm{Tr}(T_{sm}^{l}T_{sm'}^{l'+})=(2s+1)\delta_{ll'}\delta_{mm'} \tag{66c}$$

$$A=\frac{1}{2s+1}\sum_{l,m}T_{sm}^{l}\,\mathrm{Tr}(AT_{sm}^{l+}). \tag{66d}$$

Applying the results of § 2.2, one defines from the T_{sm}^{l} an irreducible Cartesian tensor T_{sl}, the only non-zero irreducible spherical components of which are the T_{sm}^{l}. The Cartesian components $(T_{sl})_{pqr}$ are then defined in terms of the basis of operators (T_{sm}^{l}) by equation (19), or, using equation (60*a*), in terms of the other basis of $\mathscr{A}_s$ $(|s\mu\rangle\langle s\mu'|)$, i.e.

$$(T_{sl})_{pqr}=\sum_{m}T_{sm}^{l}\langle lm|pqr\rangle \tag{67a}$$

$$=c^{l}\sqrt{2s+1}\sum_{m,\mu,\mu'}|s\mu\rangle\langle s\mu'|(-1)^{s-\mu'}\langle ss\mu-\mu'|lm\rangle\langle lm|pqr\rangle. \tag{67b}$$

It follows from equations (45) and (66*b*) that the operators $(T_{sl})_{pqr}$ are Hermitian:

$$(T_{sl})_{pqr}^{+}=(T_{sl})_{pqr}. \tag{68}$$

Using the orthogonality relation (49) of coefficients $\langle lm|pqr\rangle$ and equation (66*d*), one shows that any operator A in $\mathscr{A}_s$, e.g. a density operator, can be written as

$$A=\frac{1}{2s+1}\sum_{l,p,q,r}\delta_{l,p+q+r}\frac{l!}{p!q!r!}(T_{sl})_{pqr}\,\mathrm{Tr}[A(T_{sl})_{pqr}]. \tag{69}$$

Hence, the operators $(T_{sl})_{pqr}$, which are not linearly independent since they satisfy equation (20), form an overcomplete set of operators which span $\mathscr{A}_s$. Indeed, one can check, using equation (21), that they are in number

$$\sum_{l=0}^{2s}n_l=\tfrac{1}{6}(2s+1)(2s+2)(2s+3) \tag{70}$$

which is greater than the dimension $(2s+1)^2$ of $\mathscr{A}_s$ for $s>\frac{1}{2}$, the equality occurring for $s=0$ and $\frac{1}{2}$. It should be noted that the operators $(T_{sl})_{pqr}$ are non-orthogonal in the trace meaning. The expression of $(T_{sl})_{m}^{l}$ in terms of the $(T_{sl})_{pqr}$ is not unique and can be taken as the minimal expansion (24) derived in § 2.3.

3.2. Expression of tensors in terms of spin operators

Our aim now is to express the previously defined irreducible Cartesian tensors T_{sl} in terms of products of the spin operators S_x, S_y and S_z. Actually, one usually considers a multiple P_{sl} of T_{sl},

$$P_{sl}=\frac{1}{n_{sl}}T_{sl}, \tag{71}$$

with the normalisation condition

$$(P_{sl})_{00l}|ss\rangle=|ss\rangle, \tag{72}$$

from which n_{sl} is determined later in § 3.3.

One first derives the expression of the Cartesian component $(P_{sl})_{00l}$ in terms of the spin operators. It arises from equations (71), (67*b*) and (50) that

$$(P_{sl})_{00l} = c^l\sqrt{2s+1}\,\frac{\langle l0|00l\rangle}{n_{sl}}\sum_{\mu}(-1)^{s-\mu}\langle ss\mu-\mu|l0\rangle|s\mu\rangle\langle s\mu|. \tag{73}$$

Hence, $(P_{sl})_{00l}$ is diagonal in the standard basis $(|s\mu\rangle)$ and can therefore be expressed in terms of S_z only:

$$(P_{sl})_{00l} = f_{sl}(S_z). \tag{74}$$

Furthermore, the diagonal matrix elements $\langle s\mu|(P_{sl})_{00l}|s\mu\rangle$ are proportional to the Clebsch–Gordan coefficients $\langle ss\mu-\mu|l0\rangle$, the orthogonality relation of which yields

$$\sum_{\mu} f_{sl}(\mu)f_{sl'}(\mu)\propto\delta_{ll'}. \tag{75}$$

The $f_{sl}(\mu)$ are thus orthogonal polynomials of the discrete variable $\mu = s, s-1, \ldots, -s$. They are multiples of the Tchebichef polynomials (Bateman 1953) $t_l(\mu+s)$, the relevant properties of which are summed up in the appendix. It follows from the normalisation condition (72) and equation (A10) that

$$(P_{sl})_{00l} = \sum_{\lambda=0}^{[l/2]} a_{sl}^{\lambda}S_z^{l-2\lambda} = \frac{(2s-l)!}{(2s)!}t_l(S_z+s) \tag{76}$$

where $[l/2]=l/2$ or $(l-1)/2$ according to whether l is even or odd. The $(P_{sl})_{00l}$ are listed in table 4 for $l\leqslant 10$. Ohlsen (1972) gave similar results without pointing out the relation with the Tchebichef polynomials.

Let us come to the $(P_{sl})_{pqr}$ with $p+q\neq 0$. It has been noted in § 2.3 that the $(T_l)_{pqr}$ behave under the rotation group as the monomials $x^py^qz^r$, and likewise for the proportional quantities $(P_{sl})_{pqr}$. Hence, the action on $(P_{sl})_{pqr}$ of the infinitesimal generators J_i of the representation considered, here the adjoint one, cf equation (57), amounts to applying the infinitesimal generators j_i on $x^py^qz^r$. For instance, one gets with J_x

$$\begin{aligned} J_x(P_{sl})_{pqr} &\approx \frac{\mathrm{i}}{n_{sl}}\left(z\frac{\partial}{\partial y}-y\frac{\partial}{\partial z}\right)x^py^qz^r = \frac{\mathrm{i}}{n_{sl}}(qx^py^{q-1}z^{r+1}-rx^py^{q+1}z^{r-1}) \\ &= \mathrm{i}[q(P_{sl})_{p\,q-1\,r+1}-r(P_{sl})_{p\,q+1\,r-1}], \end{aligned} \tag{77}$$

and similar equations hold with J_y and J_z. It is not convenient to express the $(P_{sl})_{pqr}$ in terms of ordered products $S_x^\alpha S_y^\beta S_z^\gamma$, since the commutator of a spin operator with such a product of order $\alpha+\beta+\gamma$ generates ordered products of all orders $\leqslant\alpha+\beta+\gamma$. This is why we consider the completely symmetrical products of spin operators defined by

$$\{S_x^\alpha S_y^\beta S_z^\gamma\} = \frac{\alpha!\,\beta!\,\gamma!}{(\alpha+\beta+\gamma)!}\sum S_{i_1}\ldots S_{i_{\alpha+\beta+\gamma}}, \tag{78}$$

the sum being over the $(\alpha+\beta+\gamma)!/\alpha!\,\beta!\,\gamma!$ distinct permutations where S_x, S_y and S_z occur, respectively, α, β and γ times. The commutator of a spin operator with a symmetrised product of order $\alpha+\beta+\gamma$ can then be expressed in terms of symmetrised

Table 4. Cartesian components $(P_{sl})_{00l}$ in terms of the spin operator S_z, equation (76). The t_l are the Tchebichef polynomials of a discrete variable, equation (A1).

l	$(P_{sl})_{00l}=\sum_{\lambda=0}^{[l/2]} a_{sl}^{\lambda} S_z^{l-2\lambda}=\frac{(2s-l)!}{(2s)!}t_l(S_z+s);\ K=s(s+1)$
0	1
1	$\frac{1}{s}S_z$
2	$\frac{1}{s(2s-1)}(3S_z^2-K)$
3	$\frac{1}{s(2s-1)(s-1)}[5S_z^3-(3K-1)S_z]$
4	$\frac{1}{s(2s-1)(2s-2)(2s-3)}[5\times 7S_z^4-5(2\times 3K-5)S_z^2+3K(K-2)]$
5	$\frac{(2s-5)!}{(2s)!}2^2[3^2\times 7S_z^5-5\times 7(2K-3)S_z^3+(3\times 5K^2-2\times 5^2K+2^2\times 3)S_z]$
6	$\frac{(2s-6)!}{(2s)!}2^2[3\times 7\times 11S_z^6-3\times 5\times 7(3K-7)S_z^4+3\times 7(5K^2-5^2K+2\times 7)S_z^2$ $-5(K^3-2^3K^2+2^2\times 3K)]$
7	$\frac{(2s-7)!}{(2s)!}2^3[3\times 11\times 13S_z^7-3\times 7\times 11(3K-2\times 5)S_z^5+3\times 7(3\times 5K^2-3\times 5\times 7K+101)S_z^3$ $-(5\times 7K^3-5\times 7\times 11K^2+2\times 3^2\times 7^2K-2^2\times 3^2\times 5)S_z]$
8	$\frac{2s-8)!}{(2s)!}2[3^2\times 5\times 11\times 13S_z^8-2\times 3\times 7\times 11\times 13(2K-3^2)S_z^6$ $+3\times 5\times 7\times 11(2\times 3K^2-2^3\times 7K+3^4)S_z^4$ $-2\times 3(2\times 3\times 5\times 7K^3-3\times 5\times 7\times 29K^2+2\times 7^2\times 101K-2\times 3\times 761)S_z^2$ $+5\times 7(K^4-2^2\times 5K^3+2^2\times 3^3K^2-2^4\times 3^2K)]$
9	$\frac{(2s-9)!}{(2s)!}2^2[5\times 11\times 13\times 17S_z^9-2\times 3\times 5\times 11\times 13(2\times 3K-5\times 7)S_z^7$ $+3\times 7\times 11\times 13(2\times 3K^2-2^3\times 3^2K+5\times 29)S_z^5$ $-2\times 5\times 11(2\times 3\times 7K^3-3\times 7\times 37K^2+2\times 3^5\times 7K-2\times 5\times 263)S_z^3$ $+3(3\times 5\times 7K^4-2^2\times 5\times 7\times 19K^3+2^2\times 7\times 673K^2-2^4\times 3\times 761K+2^6\times 3\times 5\times 7)S_z]$
10	$\frac{(2s-10)!}{(2s)!}2^2[11\times 13\times 17\times 19S_z^{10}-3\times 5\times 11\times 13\times 17(3K-2\times 11)S_z^8$ $+3\times 7\times 11\times 13(2\times 3\times 5K^2-2\times 3^2\times 5^2K+11\times 109)S_z^6$ $-5\times 11\times 13(2\times 3\times 7K^3-2\times 3\times 7\times 23K^2+3^3\times 7\times 29K-2^3\times 11\times 71)S_z^4$ $+3\times 11(3\times 5\times 7K^4-2\times 5\times 7\times 47K^3$ $+2^4\times 5\times 7\times 53K^2-2^2\times 3\times 5^2\times 263K+2^4\times 3\times 11\times 61)S_z^2$ $-3^2\times 7(K^5-2^3\times 5K^4+2^2\times 127K^3-2^8\times 3^2K^2+2^6\times 3^2\times 5K)]$

products of the same order. Indeed, these products satisfy the relation (77); e.g. with J_x

$$J_x\{S_x^\alpha S_y^\beta S_z^\gamma\}=\mathrm{i}(\beta\{S_x^\alpha S_y^{\beta-1}S_z^{\gamma+1}\}-\gamma\{S_x^\alpha S_y^{\beta+1}S_z^{\gamma-1}\}). \tag{79}$$

In order to establish this result one considers the generating function

$$F_l(x,y,z)=(xS_x+yS_y+zS_z)^l=\sum_{\substack{\alpha,\beta,\gamma\\ \alpha+\beta+\gamma=l}}\frac{l!}{\alpha!\beta!\gamma!}x^\alpha y^\beta z^\gamma\{S_x^\alpha S_y^\beta S_z^\gamma\}. \tag{80}$$

One then has

$$J_xF_l(x,y,z)=\sum_{\substack{\alpha,\beta,\gamma\\ \alpha+\beta+\gamma=l}}\frac{l!}{\alpha!\beta!\gamma!}x^\alpha y^\beta z^\gamma[S_x,\{S_x^\alpha S_y^\beta S_z^\gamma\}]$$
$$=\mathrm{i}\sum_{k=0}^{l-1}(xS_x+yS_y+zS_z)^k(yS_z-zS_y)(xS_x+yS_y+zS_z)^{l-k-1}$$
$$=\mathrm{i}\sum_{\substack{\alpha',\beta',\gamma'\\ \alpha'+\beta'+\gamma'=l}}\frac{l!}{\alpha'!\beta'!\gamma'!}x^{\alpha'}y^{\beta'}z^{\gamma'}(y\{S_x^{\alpha'}S_y^{\beta'}S_z^{\gamma'+1}\}-z\{S_x^{\alpha'}S_y^{\beta'+1}S_z^{\gamma'}\}) \quad (81)$$

which yields the announced result. One should notice that the monomials in S_z which occur in equation (76) are trivially of the symmetrised type. It can now be directly checked that the expression

$$(P_{sl})_{pqr}=\sum_{\lambda=0}^{[l/2]}a_{sl}^{\lambda}\frac{(l-2\lambda)!\lambda!p!q!r!}{l!}\sum_{p'=0}^{[p/2]}\sum_{q'=0}^{[q/2]}\sum_{r'=0}^{[r/2]}\delta_{\lambda,p'+q'+r'}$$
$$\times\frac{1}{p'!q'!r'!(p-2p')!(q-2q')!(r-2r')!}\{S_x^{p-2p'}S_y^{q-2q'}S_z^{r-2r'}\} \quad (82)$$

fulfils equation (77) and coincides with the expression (76) for $p=q=0$. Therefore, it is the result we are looking for. These $(P_{sl})_{pqr}$ are given in table 5 for $l\leqslant 6$ and in table 6 for

Table 5. Cartesian components $(P_{sl})_{pqr}$ in terms of symmetrised products of spin operators, equations (78) and (82). Only the components with $p\leqslant q\leqslant r$ are listed, the other components being obtained from permutations over the indices x, y and z.

l	p	q	r	$(P_{sl})_{pqr}$
0	0	0	0	$\mathbf{1}$
1	0	0	1	$a_{s1}^0S_z$
2	0	0	2	$a_{s2}^0S_z^2+a_{s2}^1\mathbf{1}$
	0	1	1	$a_{s2}^0\{S_yS_z\}$
3	0	0	3	$a_{s3}^0S_z^3+a_{s3}^1S_z$
	0	1	2	$a_{s3}^0\{S_yS_z^2\}+\frac{1}{3}a_{s3}^1S_y$
	1	1	1	$a_{s3}^0\{S_xS_yS_z\}$
4	0	0	4	$a_{s4}^0S_z^4+a_{s4}^1S_z^2+a_{s4}^2\mathbf{1}$
	0	1	3	$a_{s4}^0\{S_yS_z^3\}+\frac{1}{2}a_{s4}^1\{S_yS_z\}$
	0	2	2	$a_{s4}^0\{S_y^2S_z^2\}+\frac{1}{6}a_{s4}^1(S_y^2+S_z^2)+\frac{1}{3}a_{s4}^2\mathbf{1}$
	1	1	2	$a_{s4}^0\{S_xS_yS_z^2\}+\frac{1}{6}a_{s4}^1\{S_xS_y\}$
5	0	0	5	$a_{s5}^0S_z^5+a_{s5}^1S_z^3+a_{s5}^2S_z$
	0	1	4	$a_{s5}^0\{S_yS_z^4\}+\frac{3}{5}a_{s5}^1\{S_yS_z^2\}+\frac{1}{5}a_{s5}^2S_y$
	0	2	3	$a_{s5}^0\{S_y^2S_z^3\}+\frac{1}{10}a_{s5}^1(3\{S_y^2S_z\}+S_z^3)+\frac{1}{5}a_{s5}^2S_z$
	1	1	3	$a_{s5}^0\{S_xS_yS_z^3\}+\frac{3}{10}a_{s5}^1\{S_xS_yS_z\}$
	1	2	2	$a_{s5}^0\{S_xS_y^2S_z^2\}+\frac{1}{10}a_{s5}^1(\{S_xS_y^2\}+\{S_xS_z^2\})+\frac{1}{15}a_{s5}^2S_x$
6	0	0	6	$a_{s6}^0S_z^6+a_{s6}^1S_z^4+a_{s6}^2S_z^2+a_{s6}^3\mathbf{1}$
	0	1	5	$a_{s6}^0\{S_yS_z^5\}+\frac{2}{3}a_{s6}^1\{S_yS_z^3\}+\frac{1}{3}a_{s6}^2\{S_yS_z\}$
	0	2	4	$a_{s6}^0\{S_y^2S_z^4\}+\frac{1}{15}a_{s6}^1(6\{S_y^2S_z^2\}+S_z^4)+\frac{1}{15}a_{s6}^2(2S_z^2+S_y^2)+\frac{1}{5}a_{s6}^3\mathbf{1}$
	1	1	4	$a_{s6}^0\{S_xS_yS_z^4\}+\frac{2}{5}a_{s6}^1\{S_xS_yS_z^2\}+\frac{1}{15}a_{s6}^2\{S_xS_y\}$
	0	3	3	$a_{s6}^0\{S_y^3S_z^3\}+\frac{1}{5}a_{s6}^1(\{S_y^3S_z\}+\{S_yS_z^3\})+\frac{1}{5}a_{s6}^2\{S_yS_z\}$
	1	2	3	$a_{s6}^0\{S_xS_y^2S_z^3\}+\frac{1}{15}a_{s6}^1(3\{S_xS_y^2S_z\}+\{S_xS_z^3\})+\frac{1}{15}a_{s6}^2\{S_xS_z\}$
	2	2	2	$a_{s6}^0\{S_x^2S_y^2S_z^2\}+\frac{1}{15}a_{s6}^1(\{S_x^2S_y^2\}+\{S_x^2S_z^2\}+\{S_y^2S_z^2\})+\frac{1}{45}a_{s6}^2(S_x^2+S_y^2+S_z^2)+\frac{1}{15}a_{s6}^3\mathbf{1}$

Table 6. Cartesian and spherical components of P_{sl}. The coefficient n_{sl} relates P_{sl} to T_{sl} according to equation (71).

s	l	n_{sl}	p	q	r	$(P_{sl})_{pqr}$	m	$c^{-l}(P_{sl})^l_m$
0	0	1	0	0	0	$\mathbf{1}$	0	$\mathbf{1}$
$\frac{1}{2}$	0	1	0	0	0	$\mathbf{1}$	0	$\mathbf{1}$
	1	1	0	0	1	$2S_z$	±1	$\mp\sqrt{2}(S_x \pm \mathrm{i}S_y)$
						$(P_{\frac{1}{2}1})_i = 2S_i$	0	$2S_z$
1	0	1	0	0	0	$\mathbf{1}$	0	$\mathbf{1}$
	1	$\sqrt{\frac{3}{2}}$	0	0	1	S_z	±1	$\mp\frac{1}{\sqrt{2}}(S_x \pm \mathrm{i}S_y)$
						$(P_{11})_i = S_i$	0	S_z
	2	$\frac{1}{\sqrt{3}}$	0	0	2	$3(S_z^2 - \frac{2}{3}\mathbf{1})$	±2	$\frac{3}{2}[S_x^2 - S_y^2 \pm \mathrm{i}(S_xS_y + S_yS_x)]$
			0	1	1	$\frac{3}{2}(S_yS_z + S_zS_y)$	±1	$\mp\frac{3}{2}[S_xS_z + S_zS_x \pm \mathrm{i}(S_yS_z + S_zS_y)]$
						$(P_{12})_{ij} = \frac{3}{2}(S_iS_j + S_jS_i) - 2\mathbf{1}\delta_{ij}$	0	$\sqrt{\frac{3}{2}}(3S_z^2 - 2\mathbf{1})$
$\frac{3}{2}$	0	1	0	0	0	$\mathbf{1}$	0	$\mathbf{1}$
	1	$\frac{3}{\sqrt{5}}$	0	0	1	$\frac{2}{3}S_z$	±1	$\mp\frac{\sqrt{2}}{3}(S_x \pm \mathrm{i}S_y)$
						$(P_{\frac{3}{2}1})_i = \frac{2}{3}S_i$	0	$\frac{2}{3}S_z$
	2	$\sqrt{\frac{2}{3}}$	0	0	2	$S_z^2 - \frac{5}{4}\mathbf{1}$	±2	$\frac{1}{2}[S_x^2 - S_y^2 \pm \mathrm{i}(S_xS_y + S_yS_x)]$
			0	1	1	$\frac{1}{2}(S_yS_z + S_zS_y)$	±1	$\mp\frac{1}{2}[S_xS_z + S_zS_x \pm \mathrm{i}(S_yS_z + S_zS_y)]$
						$(P_{\frac{3}{2}2})_{ij} = \frac{1}{2}(S_iS_j + S_jS_i) - \frac{5}{4}\mathbf{1}\delta_{ij}$	0	$\sqrt{\frac{3}{2}}(S_z^2 - \frac{5}{4}\mathbf{1})$
	3	$\frac{\sqrt{2}}{5}$	0	0	3	$\frac{10}{3}(S_z^3 - \frac{41}{20}S_z)$	±3	$\mp\frac{5}{3\sqrt{2}}[S_x^3 - 3S_yS_xS_y - S_x \mp \mathrm{i}(S_y^3 - 3S_xS_yS_x - S_y)]$
			0	1	2	$\frac{10}{3}(S_zS_yS_z - \frac{7}{20}S_y)$	±2	$\frac{5}{\sqrt{3}}[S_xS_zS_x - S_yS_zS_y \pm \mathrm{i}(S_xS_yS_z + S_zS_yS_x)]$
			1	1	1	$\frac{5}{3}(S_xS_yS_z + S_zS_yS_x)$	±1	$\mp5\sqrt{\frac{5}{6}}[S_zS_xS_z - \frac{7}{20}S_x \pm \mathrm{i}(S_zS_yS_z - \frac{7}{20}S_y)]$
						$(P_{\frac{3}{2}3})_{ijk} = \frac{5}{3}[S_iS_jS_k + S_kS_jS_i - \frac{17}{10}(S_i\delta_{jk} + S_k\delta_{ij}) - \frac{7}{10}S_j\delta_{ik}]$	0	$\frac{5}{3}\sqrt{10}(S_z^3 - \frac{41}{20}S_z)$

s	l	n_{sl}	p	q	r	$(P_{sl})_{pqr}$	m	$c^{-l}(P_{sl})^l_m$
2	0	1	0	0	0	$\mathbf{1}$	0	$\mathbf{1}$
	1	$\sqrt{2}$	0	0	1	$\frac{1}{2}S_z$	±1	$\mp\frac{1}{2\sqrt{2}}(S_x \pm \mathrm{i}S_y)$
						$(P_{21})_i = \frac{1}{2}S_i$	0	$\frac{1}{2}S_z$
	2	$2\sqrt{\frac{5}{21}}$	0	0	2	$\frac{1}{2}(S_z^2 - 2\mathbf{1})$	±2	$\frac{1}{4}[S_x^2 - S_y^2 \pm \mathrm{i}(S_xS_y + S_yS_x)]$
			0	1	1	$\frac{1}{4}(S_yS_z + S_zS_y)$	±1	$\mp\frac{1}{4}[S_xS_z + S_zS_x \pm \mathrm{i}(S_yS_z + S_zS_y)]$
						$(P_{21})_{ij} = \frac{1}{4}(S_iS_j + S_jS_i) - \mathbf{1}\delta_{ij}$	0	$\frac{1}{2}\sqrt{\frac{3}{2}}(S_z^2 - 2\mathbf{1})$
	3	$\frac{1}{\sqrt{5}}$	0	0	3	$\frac{5}{6}(S_z^3 - \frac{17}{5}\mathbf{1})$	±3	$\mp\frac{5}{12\sqrt{2}}[S_x^3 - 3S_yS_xS_y - S_x \mp \mathrm{i}(S_y^3 - 3S_xS_yS_x - S_y)]$
			0	1	2	$\frac{5}{6}(S_zS_yS_z - \frac{4}{5}S_y)$	±2	$\frac{5}{4\sqrt{3}}[S_xS_zS_x - S_yS_zS_y \pm \mathrm{i}(S_xS_yS_z + S_zS_yS_x)]$
			1	1	1	$\frac{5}{12}(S_xS_yS_z + S_zS_yS_x)$	±1	$\mp\frac{5}{4}\sqrt{\frac{5}{6}}[S_zS_xS_z - \frac{4}{5}S_x \pm \mathrm{i}(S_zS_yS_z - \frac{4}{5}S_y)]$
						$(P_{23})_{ijk} = \frac{5}{12}[S_iS_jS_k + S_kS_jS_i - \frac{13}{5}(S_i\delta_{jk} + S_k\delta_{ij}) - \frac{8}{5}S_j\delta_{ik}]$	0	$\frac{5}{6}\sqrt{\frac{5}{2}}(S_z^3 - \frac{17}{5}S_z)$
	4	$\frac{2}{7\sqrt{5}}$	0	0	4	$\frac{35}{12}(S_z^4 - \frac{31}{7}S_z^2 + \frac{72}{35}\mathbf{1})$	±4	$\frac{35}{48}[S_x^4 + S_y^4 - 3(S_x^2S_y^2 + S_y^2S_x^2) + 2(S_x^2 + S_y^2)$
								$- 3S_z^2 \pm 2\mathrm{i}(S_x^3S_y + S_yS_x^3 - S_xS_y^3 - S_y^3S_x)]$
			0	1	3	$\frac{35}{24}[S_yS_z^3 + S_z^3S_y - \frac{19}{7}(S_yS_z + S_zS_y)]$	±3	$\mp\frac{35}{24\sqrt{2}}\{S_x^3S_z + S_zS_x^3 - 3(S_xS_zS_y^2 + S_y^2S_zS_x) + 2(S_xS_z + S_zS_x)$
			0	2	2	$\frac{35}{24}[S_y^2S_z^2 + S_z^2S_y^2 - \frac{15}{7}(S_y^2 + S_z^2) + S_x^2 + \frac{48}{35}\mathbf{1}]$		$\mp\mathrm{i}[S_y^3S_z + S_zS_y^3 - 3(S_zS_yS_x^2 + S_x^2S_yS_z) + 2(S_yS_z + S_zS_y)]\}$
			1	1	2	$\frac{35}{24}[S_xS_yS_z^2 + S_z^2S_yS_x - \frac{97}{42}(S_xS_y + S_yS_x)]$	±2	$\frac{35}{48}\sqrt{7}\{S_x^2S_z^2 + S_z^2S_x^2 - S_y^2S_z^2 - S_z^2S_y^2 - \frac{22}{7}(S_x^2 - S_y^2)$
								$\pm\mathrm{i}[2(S_xS_yS_z^2 + S_z^2S_yS_x) - \frac{22}{7}(S_xS_y + S_yS_x)]\}$
							±1	$\mp\frac{35}{24}\sqrt{\frac{7}{2}}\{S_xS_z^3 + S_z^3S_x - \frac{19}{7}(S_xS_z + S_zS_x)$
								$\pm\mathrm{i}[S_yS_z^3 + S_z^3S_y - \frac{19}{7}(S_yS_z + S_zS_y)]\}$
							0	$\frac{35}{24}\sqrt{\frac{35}{2}}(S_z^4 - \frac{31}{7}S_z^2 + \frac{72}{35}\mathbf{1})$

$s \leqslant 2$. Using the initial notation of Cartesian components, i.e. $(P_{sl})_{i_1 \ldots i_l}$, one has, for instance,

$$P_{s0} = \mathbf{1} \tag{83a}$$

$$(P_{s1})_i = a^0_{s1} S_i \tag{83b}$$

$$(P_{s2})_{ij} = a^0_{s2}\{S_i S_j\} + a^1_{s2} \mathbf{1} \delta_{ij} \tag{83c}$$

$$(P_{s3})_{ijk} = a^0_{s3}\{S_i S_j S_k\} + \tfrac{1}{3} a^1_{s3}(S_i\delta_{jk} + S_j\delta_{ik} + S_k\delta_{ij}). \tag{83d}$$

These expressions can be simplified thanks to the commutation relations of spin operators, cf tables 6–8, and, for example,

$$(P_{s3})_{ijk} = \tfrac{1}{2} a^0_{s3}(S_i S_j S_k + S_k S_j S_i) - \tfrac{1}{6}(a^0_{s3} - 2a^1_{s3})(S_i\delta_{jk} + S_k\delta_{ij}) + \tfrac{1}{3}(a^0_{s3} + a^1_{s3}) S_j \delta_{ik} \tag{84}$$

which is different from the formula given by Keaton (1971) for $s = \frac{3}{2}$ ($a^0_{3/2\,3} = \frac{10}{3}$, $a^1_{3/2\,3} = -\frac{41}{6}$; its expression is not completely symmetrical with respect to the three Cartesian indices). It should be noticed that the relation (56*b*) allows us to modify the expressions in terms of the spin operators.

3.3. Properties of Cartesian and spherical components of tensors P_{sl}

As for the T_{sl} to which they are proportional, the tensors P_{sl} are traceless on contraction of any pair of Cartesian indices, i.e. from equation (20)

$$(P_{sl})_{p'+2\,q'r'} + (P_{sl})_{p'q'+2\,r'} + (P_{sl})_{p'q'r'+2} = 0 \qquad p' + q' + r' = l - 2. \tag{85}$$

It must be possible to check this property using the general formula (82), equation (56*b*), and taking care of the symmetrised character of products of spin operators. We only check equation (85) for the special cases given in table 5.

The normalisation factor n_{sl} can be obtained up to a sign from the orthogonality relations of the Tchebichef polynomials, equation (A3), and of the operators $(T_{sl})^l_m$, equation (66*c*). Its sign then follows from the relative sign between any same matrix element of $(P_{sl})^l_m$ and $(T_{sl})^l_m$. However, this normalisation factor arises directly from the relation (A8*b*) between the Tchebichef polynomial $t_l(\mu + s)$ and the Clebsch–Gordan coefficient $\langle ss\mu - \mu | l0 \rangle$. On comparing the values of the matrix element $\langle s\mu | (P_{sl})_{00l} | s\mu \rangle$ which arises from equations (50), (73) and (76) one finds

$$n_{sl} = (2s)!\,l!\left(\frac{(2s+1)(2l+1)2^l}{(2s-l)!(2s+l+1)!(2l)!}\right)^{1/2}. \tag{86}$$

The values of this factor are listed in table 6 for $s \leqslant 2$. Since n_{sl} is real and the $(T_{sl})_{pqr}$ are Hermitian operators, equation (68), we get

$$(P_{sl})^+_{pqr} = (P_{sl})_{pqr} \tag{87}$$

as also follows from the general formula (82). From equations (69), (71) and (86) any operator A in $\mathscr{A}_s$ can be written as

$$A = [(2s)!]^2 \sum_{l,p,q,r} \delta_{l,p+q+r} \frac{(2l+1)2^l(l!)^3}{p!\,q!\,r!\,(2s-l)!(2s+l+1)!(2l)!} (P_{sl})_{pqr}\, \mathrm{Tr}[A(P_{sl})_{pqr}]. \tag{88}$$

As for the $(T_{sl})_{pqr}$, the $(P_{sl})_{pqr}$ thus form an overcomplete system of non-orthogonal Hermitian operators which span $\mathscr{A}_s$.

As for the irreducible Cartesian tensor T_{sl}, the expression for the spherical components of P_{sl} in terms of its Cartesian components is not unique and can be taken as the minimal expansion (24):

$$(P_{sl})^l_m = \sum_{\substack{p,q,r \\ p+q+r=l}} (P_{sl})_{pqr}(pqr|lm). \tag{89}$$

Expressing the $(P_{sl})_{pqr}$ by equation (82), one then obtains the $(P_{sl})^l_m$ in terms of the spin operators. This result for $l \leqslant 4$ can be obtained by replacing in table 1 the monomials $x^p y^q z^r$ by the $(P_{sl})_{pqr}$ listed in table 5. One thereby finds the expressions given in table 6 for $s \leqslant 2$ and in table 7 for $l \leqslant 4$. In terms of the spherical components $(P_{sl})^l_m$, the

Table 7. Spherical components $(P_{sl})^l_m$, equation (89), in terms of spin operators.

l	m	$c^{-l}(P_{sl})^l_m$
0	0	$\mathbf{1}$
1	±1	$\mp\frac{1}{\sqrt{2}}a^0_{s1}(S_x \pm \mathrm{i}S_y)$
	0	$a^0_{s1}S_z$
2	±2	$\frac{1}{2}a^0_{s2}[S_x^2 \pm \mathrm{i}(S_xS_y + S_yS_x) - S_y^2]$
	±1	$\mp\frac{1}{2}a^0_{s2}[S_xS_z + S_zS_x \pm \mathrm{i}(S_yS_z + S_zS_y)]$
	0	$\sqrt{\frac{3}{2}}(a^0_{s2}S_z^2 + a^1_{s2}\mathbf{1})$
3	±3	$\mp\frac{1}{2\sqrt{2}}a^0_{s3}[S_x^3 - 3S_yS_xS_y - S_x \mp \mathrm{i}(S_y^3 - 3S_xS_yS_x - S_y)]$
	±2	$\frac{\sqrt{3}}{2}a^0_{s3}[S_xS_zS_x - S_yS_zS_y \pm \mathrm{i}(S_xS_yS_z + S_zS_yS_x)]$
	±1	$\mp\frac{1}{2}\sqrt{\frac{15}{2}}\{a^0_{s3}S_zS_xS_z + \frac{1}{3}(a^0_{s3} + a^1_{s3})S_x \pm \mathrm{i}[a^0_{s3}S_zS_yS_z + \frac{1}{3}(a^0_{s3} + a^1_{s3})S_y]\}$
	0	$\sqrt{\frac{5}{2}}(a^0_{s3}S_z^3 + a^1_{s3}S_z)$
4	±4	$\frac{1}{4}a^0_{s4}[S_x^4 + S_y^4 - 3(S_x^2S_y^2 + S_y^2S_x^2) + 2(S_x^2 + S_y^2) - 3S_z^2 \pm 2\mathrm{i}(S_x^3S_y + S_yS_x^3 - S_xS_y^3 - S_y^3S_x)]$
	±3	$\mp\frac{1}{2\sqrt{2}}a^0_{s4}\{S_x^3S_z + S_zS_x^3 - 3(S_xS_zS_y^2 + S_y^2S_zS_x) + 2(S_xS_z + S_zS_x)$
		$\mp\mathrm{i}[S_y^3S_z + S_zS_y^3 - 3(S_zS_yS_x^2 + S_x^2S_yS_z) + 2(S_yS_z + S_zS_y)]\}$
	±2	$\frac{\sqrt{7}}{4}\{a^0_{s4}(S_x^2S_z^2 + S_z^2S_x^2 - S_y^2S_z^2 - S_z^2S_y^2) - \frac{1}{3}(5a^0_{s4} - a^1_{s4})(S_x^2 - S_y^2)$
		$\pm\mathrm{i}[2a^0_{s4}(S_xS_yS_z^2 + S_z^2S_yS_x) - \frac{1}{3}(5a^0_{s4} - a^1_{s4})(S_xS_y + S_yS_x)]\}$
	±1	$\mp\frac{1}{2}\sqrt{\frac{7}{2}}\{a^0_{s4}(S_xS_z^3 + S_z^3S_x) - \frac{1}{2}(a^0_{s4} - a^1_{s4})(S_xS_z + S_zS_x)$
		$\pm\mathrm{i}[a^0_{s4}(S_yS_z^3 + S_z^3S_y) - \frac{1}{2}(a^0_{s4} - a^1_{s4})(S_yS_z + S_zS_y)]\}$
	0	$\frac{1}{2}\sqrt{\frac{35}{2}}(a^0_{s4}S_z^4 + a^1_{s4}S_z^2 + a^2_{s4}\mathbf{1})$

properties (66*a–d*) read

$$(P_{s0})^0_0 = \mathbf{1} \tag{90a}$$

$$(P_{sl})^{l+}_m = c^{-2l}(-1)^m(P_{sl})^l_{-m} \tag{90b}$$

$$\mathrm{Tr}[(P_{sl})^l_m(P_{sl'})^{l'+}_{m'}] = \frac{(2s-l)!(2s+l+1)!(2l)!}{(2l+1)2^l[(2s)!l!]^2}\delta_{ll'}\delta_{mm'} \tag{90c}$$

$$A = [(2s)!]^2 \sum_{l,m} \frac{(2l+1)2^l(l!)^2}{(2s-l)!(2s+l+1)!(2l)!}(P_{sl})^l_m \,\mathrm{Tr}[A(P_{sl})^{l+}_m]. \tag{90d}$$

Hence, the $(P_{sl})^l_m$ form an orthogonal basis of operators in terms of which any operator in $\mathscr{A}_s$ can be expressed according to equation (90*d*).

Instead of the bases of operators $(T_{sl})^l_m$ or $(P_{sl})^l_m$, one can consider the other basis of operators $\{A^1_{sl0}, A^\varepsilon_{slm};\ l = 0, \ldots, 2s,\ m = 1, \ldots, l,\ \varepsilon = \pm1\}$ defined by equation (52), adding a subscript s, or the proportional operators

$$C_{slm} = \frac{1}{n_{sl}} A^{\varepsilon}_{slm} = \frac{1}{1+\delta_{m0}} \left(\frac{2^l (l-m)!(l+m)!}{(2l)!} \right)^{1/2} [(P_{sl})^l_m + \varepsilon (P_{sl})^l_{-m}]. \qquad (91)$$

Using equation (90b), their Hermitian conjugate reads

$$C^{\varepsilon +}_{slm} = c^{-2l}(-1)^m \varepsilon C^{\varepsilon}_{slm}, \qquad (92)$$

and equation (90c) yields the orthogonality relation

$$\mathrm{Tr}(C^{\varepsilon}_{slm} C^{\varepsilon' +}_{sl'm'}) = \frac{2}{1+\delta_{m0}} \frac{(l-m)!(l+m)!(2s-l)!(2s+l+1)!}{(2l+1)[(2s)!l!]^2} \delta_{\varepsilon\varepsilon'} \delta_{ll'} \delta_{mm'} \qquad (93)$$

for all non-negative m and m'. Therefore, any operator A in $\mathscr{A}_s$ can be written as

$$A = [(2s)!]^2 \sum_{l=0}^{2s} \sum_{m=0}^{l} \sum_{\varepsilon=\pm 1} \frac{1+\delta_{m0}}{2} \times \frac{(2l+1)(l!)^2}{(l-m)!(l+m)!(2s-l)!(2s+l+1)!} C^{\varepsilon}_{slm} \, \mathrm{Tr}(A C^{\varepsilon +}_{slm}) \qquad (94)$$

where $\varepsilon = 1$ if $m = 0$. It follows from equation (53) that the C^{ε}_{slm} read, in terms of the Cartesian components $(P_{sl})_{pqr}$,

$$C^{\varepsilon}_{slm} = c^l (-1)^m \sum_{\mu=0}^{m} \mathrm{i}^{\mu} \binom{m}{\mu} \frac{1+\varepsilon(-1)^{m+\mu}}{1+\delta_{m0}} (P_{sl})_{m-\mu \; \mu \; l-m}. \qquad (95)$$

The two equations above provide us with a minimal expansion of any operator A in $\mathscr{A}_s$ in terms of Cartesian component operators. Namely, any A is then expressed in terms of $(2s+1)^2$ linearly independent linear combinations of the $(P_{sl})_{pqr}$. Actually, instead of the C^{ε}_{slm}, one usually considers the quantities

$$D^{\varepsilon +}_{slm} \approx B^{\varepsilon}_{m} z^{l-m} \qquad (96)$$

where the B^{ε}_m are defined by equations (54b–e) and $\approx$ means that each monomial $x^p y^q z^r$ here stands for $(P_{sl})_{pqr}$. The C^{ε}_{slm} and the D^{ε}_{slm} are then related by equation (54a) replacing A^{ε}_{lm} and $B^{\varepsilon}_{m} z^{l-m}$ by C^{ε}_{slm} and D^{ε}_{slm}, respectively. Using tables 3–5, the expressions for the D^{ε}_{slm} in terms of the spin operators are listed in table 8 for $l \leqslant 4$. The operators $\{D^1_{sl0}, D^{\varepsilon}_{slm};\, l = 0, \ldots, 2s,\, m = 1, \ldots, l,\, \varepsilon = \pm 1\}$ are Hermitian,

$$D^{\varepsilon +}_{slm} = D^{\varepsilon}_{slm}, \qquad (97)$$

and form another orthogonal basis of $\mathscr{A}_s$ in terms of which any operator A reads as the minimal expansion

$$\begin{aligned} A = [(2s)!]^2 \sum_{l=0}^{2s} \frac{(2l+1)(l!)^2}{(2s-l)!(2s+l+1)!} \Bigg\{ & \sum_{n=0}^{[l/2]} \frac{2}{1+\delta_{n0}} \frac{1}{(l-2n)!(l+2n)!} \\ & \times [D^1_{sl2n} \, \mathrm{Tr}(A D^1_{sl2n}) + 4n^2 D^{-1}_{sl2n} \, \mathrm{Tr}(A D^{-1}_{sl2n})] \\ & + \sum_{n=0}^{[(l-1)/2]} \frac{2}{(l-2n-1)!(l+2n+1)!} \\ & \times [D^1_{sl2n+1} \, \mathrm{Tr}(A D^1_{sl2n+1}) + D^{-1}_{sl2n+1} \, \mathrm{Tr}(A D^{-1}_{sl2n+1})] \Bigg\}. \end{aligned} \qquad (98)$$

Table 8. Operators D^{ε}_{slm}, equation (96), in terms of spin operators. The factor a^0_{sl} is the coefficient of the highest degree symmetrised monomial $\{S^p_x S^q_y S^r_z\}$ in $(P_l)_{pqr}$ which follows from equation (A11).

l	m	ε	$a^0_{sl} = \dfrac{(2s-l)!(2l)!}{(2s)!(l!)^2}$	$\dfrac{1}{a^0_{sl}} D^{\varepsilon}_{slm};\ K = s(s+1)$
0	0	1	1	1
1	1	1	$\dfrac{1}{s}$	S_y
		−1		S_x
	0	1		S_z
2	2	1	$\dfrac{3}{s(2s-1)}$	$S_x^2 - S_y^2$
		−1		$\{S_xS_y\} = \frac{1}{2}(S_xS_y + S_yS_x)$
	1	1		$\{S_yS_z\} = \frac{1}{2}(S_yS_z + S_zS_y)$
		−1		$\{S_xS_z\} = \frac{1}{2}(S_xS_z + S_zS_x)$
	0	1		S_z^3
3	3	1	$\dfrac{5}{s(2s-1)(s-1)}$	$S_y^3 - 3\{S_x^2S_y\} = S_y^3 - 3S_sS_yS_x - S_y$
		−1		$S_x^3 - 3\{S_xS_y^2\} = S_x^3 - 3S_yS_xS_y - S_x$
	2	1		$\{S_x^2S_z\} - \{S_y^2S_z\} = S_xS_zS_x - S_yS_zS_y$
		−1		$\{S_xS_yS_z\} = \frac{1}{2}(S_xS_yS_z + S_zS_yS_x)$
	1	1		$\{S_yS_z^2\} - \frac{1}{15}(3K-1)S_y = S_zS_yS_z - \frac{1}{5}(K-2)S_y$
		−1		$\{S_xS_z^2\} - \frac{1}{15}(3K-1)S_x = S_zS_xS_z - \frac{1}{5}(K-2)S_x$
	0	1		S_z^3
4	4	1	$\dfrac{35}{s(2s-1)(2s-2)(2s-3)}$	$S_x^4 - 6\{S_x^2S_y^2\} + S_y^4$
		−1		$\{S_x^3S_y\} - \{S_xS_y^3\}$
	3	1		$\{S_y^3S_z\} - 3\{S_x^2S_yS_z\}$
		−1		$\{S_x^3S_z\} - 3\{S_xS_y^2S_z\}$
	2	1		$\{S_x^2S_z^2\} - \{S_y^2S_z^2\} - \frac{1}{42}(6K-5)(S_x^2 - S_y^2)$
		−1		$\{S_xS_yS_z^2\} - \frac{1}{42}(6K-5)\{S_xS_y\}$
	1	1		$\{S_yS_z^3\} - \frac{1}{14}(6K-5)\{S_yS_z\}$
		−1		$\{S_xS_z^3\} - \frac{1}{14}(6K-5)\{S_xS_z\}$
	0	1		S_z^4

Using the simplified notation

$$A^{s}_{pqr} = \mathrm{Tr}[A(P_{sl})_{pqr}] \tag{99}$$

and table 3, we get explicitly for $l \leqslant 4$

$$A = \frac{1}{2s+1}\Bigg(\mathrm{Tr}\,A + \frac{3s}{s+1}[(P_{s1})_{100}A^{s}_{100} + (P_{s1})_{010}A^{s}_{010} + (P_{s1})_{001}A^{s}_{001}]$$

$$+\frac{5s(2s-1)}{(s+1)(2s+3)}\{\tfrac{1}{3}[(P_{s2})_{200} - (P_{s2})_{020}](A^{s}_{200} - A^{s}_{020})$$

$$+\tfrac{4}{3}[(P_{s2})_{110}A^{s}_{110} + (P_{s2})_{101}A^{s}_{101} + (P_{s2})_{011}A^{s}_{011}] + (P_{s2})_{002}A^{s}_{002}\}$$

$$+\frac{7s(2s-1)(s-1)}{(s+1)(2s+3)(s+2)}\{\tfrac{1}{10}[(P_{s3})_{003} - 3(P_{s3})_{120}](A^{s}_{003} - 3A^{s}_{120})$$

$$+\tfrac{1}{10}[(P_{s3})_{030}-3(P_{s2})_{210}](A^s_{030}-3A^s_{210})+\tfrac{3}{5}[(P_{s3})_{201}-(P_{s3})_{021}](A^s_{201}$$
$$-A^s_{021})+\tfrac{12}{5}(P_{s3})_{111}A^s_{111}+\tfrac{3}{2}[(P_{s3})_{102}A^s_{102}+(P_{s3})_{012}A^s_{012}]+(P_{s3})_{003}A^s_{003}\}$$
$$+\frac{9s(2s-1)(s-1)(2s-3)}{(s+1)(2s+3)(s+2)(2s+5)}\{\tfrac{1}{35}[(P_{s4})_{400}-6(P_{s4})_{220}+(P_{s4})_{040}]$$
$$\times(A^s_{400}-6A^s_{220}+A^s_{040})+\tfrac{16}{35}[(P_{s4})_{310}-(P_{s4})_{130}](A^s_{310}-A^s_{130})$$
$$+\tfrac{8}{35}[(P_{s4})_{031}-3(P_{s4})_{211}](A^s_{031}-3A^s_{211})$$
$$+\tfrac{8}{35}[(P_{s4})_{301}-3(P_{s4})_{121}](A^s_{301}-3A^s_{121})$$
$$+\tfrac{4}{5}[(P_{s4})_{202}-(P_{s4})_{022}](A^s_{202}-A^s_{022})$$
$$+\tfrac{16}{5}(P_{s4})_{112}A^s_{112}+\tfrac{8}{5}[(P_{s4})_{103}A^s_{103}+(P_{s4})_{013}A^s_{013}]$$
$$+(P_{s4})_{004}A^s_{004}\}+\sum_{l=5}^{2s}\ldots\Big). \tag{100}$$

4. Conclusion

In practice, any operator in $\mathcal{A}_s$ is expanded either in terms of the spherical component operators $(T_{sl})^l_m$, equation (66d), or in terms of the Cartesian component operators $(P_{sl})_{pqr}$, equation (88). The first expansion is over an orthogonal basis of operators and the only coefficient, i.e. $(2s+1)$, arises from the choice of unity as $(T_{s0})^0_0$. On the other hand, the second expansion is over a superfluous set of non-orthogonal operators and, furthermore, the coefficients have a non-trivial s and l dependence. Taking into account the relation (85) between the $(P_{sl})_{pqr}$, one can extract from this overcomplete set of operators different bases defined by linear combinations of the $(P_{sl})_{pqr}$. A simple way to do this is given by the minimal expansion (98), and more explicitly by equation (100). This third expansion of any operator is closely related to the first one discussed above, but the coefficients are even more complicated than in the second expansion since they are all different.

The Cartesian component operators and the spherical component operators for $c=1$ coincide with the operators adopted in the Madison convention (1971) for the description of nuclear reactions involving spin-$\frac{1}{2}$ and spin-1 particles. For this type of application and with the choice of coordinate system specified in the convention quoted above, the parity conservation leads us to consider density operators ρ which are symmetrical with respect to the $x0z$ plane. One then has

$$\rho^s_{lm}=\mathrm{Tr}[\rho(T_{sl})^l_m]=(-1)^{l-m}\rho^s_{l-m} \tag{101a}$$

$$\rho^s_{pqr}=\mathrm{Tr}[\rho(T_{sl})_{pqr}]=0 \qquad \text{if } p+r \text{ odd} \tag{101b}$$

$$\rho^{s\varepsilon}_{lm}=\mathrm{Tr}[\rho D^\varepsilon_{slm}]=0 \qquad \text{if } (-1)^{l-m}\neq\varepsilon. \tag{101c}$$

To study the azimuthal dependence of a reaction one needs to know how the three types of basis operators depend upon the change of coordinate systems, i.e. a rotation of φ about the z axis. Let us specify by the index φ the quantities defined with respect to the rotated coordinate system. For the first and the third bases one has

$${}^{\varphi}(T_{sl})^l_m=\mathrm{e}^{-\mathrm{i}m\varphi}(T_{sl})^l_m \tag{102a}$$

$${}^{\varphi}D^\varepsilon_{slm}=(\cos m\varphi)D^\varepsilon_{slm}+(\sin m\varphi)g^\varepsilon_m D^{-\varepsilon}_{slm} \tag{102b}$$

where the value of $g^{\varepsilon}_m = -\mathrm{i}f^{-\varepsilon}_m/f^{\varepsilon}_m$ follows from equations (54*b*–*e*):

$$g^{1}_{2n} = 2n \qquad g^{-1}_{2n} = -\frac{1}{2n} \qquad g^{1}_{2n+1} = (-1)^{n+1} \qquad g^{-1}_{2n+1} = (-1)^{n}. \tag{103}$$

For the Cartesian component operators the expressions are more complicated, since they are given by

$$^{\varphi}(P_{sl})_{pqr} \approx (x\cos\varphi + y\sin\varphi)^{p}(-x\sin\varphi + y\cos\varphi)^{q}z^{r} \tag{104}$$

where $\approx$ means that $x^{p}y^{q}z^{r}$ stands for $(P_{sl})_{pqr}$. It should be noticed that in the first and third cases the different values of m are not mixed under this rotation, while in the second case all values of p' and q' such that $p+q=p'+q'$ are generated. From all these considerations, the use of the spherical component operators $(T_{sl})^{l}_{m}$ appears to be the most convenient one.

As far as the use of the spin operators is concerned, we have given general formulae for the considered basis operators in terms of symmetrised products, equation (78). However, the expressions for these latter products involve many terms.

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Appendix. Tchebichef's polynomials of a discrete variable

The Tchebichef polynomials $t_n(x)$, as defined by Bateman (1953), are the orthogonal polynomials with the weight function 1 of the discrete variable $x = 0, 1, \ldots, N-1$. One here considers the case

$$N = 2s+1 \qquad n = l \qquad x = \mu + s \qquad \mu = s, s-1, \ldots, -s.$$

Let us then sum up the properties of the polynomials $t_l(\mu+s)$ in which we are interested.

Definition:

$$t_l(\mu+s) = l!\,\Delta^{l}\left[\binom{\mu+s}{l}\binom{\mu-s-1}{l}\right] \qquad l = 0, 1, \ldots, 2s \tag{A1}$$

where

$$\Delta f(\mu) = f(\mu+1) - f(\mu) \qquad \Delta^{n+1}f(\mu) = \Delta[\Delta^{n}f(\mu)]. \tag{A2}$$

Orthogonality relation:

$$\sum_{\mu=-s}^{s} t_l(\mu+s)t_{l'}(\mu+s) = \frac{(2s+l+1)!}{(2l+1)(2s-l)!}\delta_{ll'}. \tag{A3}$$

Difference equation:

$$(\mu+s+2)(\mu-s+1)\Delta^2 t_l(\mu+s)+[2\mu+2-l(l+1)]\Delta t_l(\mu+s)-l(l+1)t_l(\mu+s)=0. \tag{A4}$$

Recurrence formula:

$$(l+1)t_{l+1}(\mu+s)-2(2l+1)\mu t_l(\mu+s)+l[(2s+1)^2-l^2]t_{l-1}(\mu+s)=0$$
$$l=1,2,\ldots,2s-1. \tag{A5}$$

Symmetry property. Parity in μ:

$$t_l(\mu+s)=(-1)^l t_l(-\mu+s). \tag{A6}$$

Relation with the generalised hypergeometric function ${}_3F_2$:

$$t_l(\mu+s)=(-1)^l\frac{(2s)!}{(2s-l)!}{}_3F_2(-l,-\mu-s,1+l;1,-2s;1). \tag{A7}$$

Relation with a Clebsch–Gordan coefficient. From the equation above and equation (22) of Varshalovich *et al* (1975) one has

$$t_l(\mu+s)=(-1)^l\left(\frac{(2s+l+1)!}{(2s+1)(2s-l)!}\right)^{1/2}\langle ls0\mu|s\mu\rangle \tag{A8a}$$

$$=(-1)^{s-\mu}\left(\frac{(2s+l+1)!}{(2l+1)(2s-l)!}\right)^{1/2}\langle ss\mu-\mu|l0\rangle. \tag{A8b}$$

Special values:

$$t_l(s)=\begin{cases}(-1)^{l/2}l!\binom{l}{l/2}\binom{s+l/2}{l/2} & l \text{ even}\\ 0 & l \text{ odd}\end{cases} \tag{A9}$$

$$t_l(2s)=\frac{(2s)!}{(2s-l)!}. \tag{A10}$$

Coefficient of the highest power in μ:

$$t_l(\mu+s)=\frac{(2l)!}{(l!)^2}\mu^l+O(\mu^{l-2}). \tag{A11}$$

Special cases. The $t_l(\mu+s)$ are listed in table 4 for $l\leqslant 10$.

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